

Nano-clusters: At What Point does Metallic Magnesium Become Non-Metallic?

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Experimental and theoretical studies of the non-metallic-to-metallic transition in magnesium cluster anions, Mg_n^- , have found the onset of metallicity to occur at $n = 18$. These results mark the first time that the gap between the binding energies of the two most external electrons in anionic clusters, which is the finite-size analog of the gap between the valence and the conduction bands of the bulk, has actually been seen to close in metal clusters. Kit Bowen of Johns Hopkins University (Chemistry Dept.) and Julius Jellinek of Argonne National Laboratory (Chemistry Division) have conducted separate but complementary investigations into this problem. Bowen's contribution was to measure the anion photoelectron spectra of these species, while Jellinek's contribution was to compute many of the same quantities measured in the experiment. The agreement between these studies is excellent, each part enhancing physical insight into the other. Recently, their articles were accepted for back-to-back publication in Physical Review Letters. Bowen's work is supported by the Division of Materials Science (BES), while Jellinek's work is supported by the Division of Chemical Sciences, Geosciences, & Biosciences (BES).

Gap Between the Binding Energies of the Two Most External Electrons in Anionic Magnesium Clusters

